

REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-09-0151

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1. REPORT DATE (DD-MM-YYYY) 30-04-2009		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 01-02-2006 though 31-01-2009	
4. TITLE AND SUBTITLE Spectroscopy and Dynamics of Transient and Energetic Species				5a. CONTRACT NUMBER FA9550-06-1-0085	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
				5d. PROJECT NUMBER	
6. AUTHOR(S) Daniel M. Neumark				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research Dr. Michael R. Berman / <i>NA</i> 875 North Randolph Street Suite 325, Room 3112 Arlington, VA 22203				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) FA9550-06-1-0085	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release/distribution is unlimited					
13. SUPPLEMENTARY NOTES None.					
14. ABSTRACT Free radicals, weakly bound van der Waals complexes, and metal and semi-conductor clusters are characterized by photodetachment of the corresponding negative ions using slow electron velocity-map imaging (SEVI), a recently developed, high-resolution (2-3 cm-1) variant of negative ion photoelectron spectroscopy. The SEVI spectrum of a negative ion yields the electron affinity of the neutral, term values for excited states accessible via one-photon detachment, and accurate vibrational frequencies for the ground and accessible excited states. The combination of high energy resolution and the simultaneous measurement of photoelectron angular distributions provides a sensitive probe of adiabatic potential energy surfaces and vibronic coupling in neutral species formed by photodetachment. The SEVI experiments are complemented by infrared studies of size-selected negative ions and clusters using the free electron laser FELIX.					
15. SUBJECT TERMS negative ion, photodetachment, and photodissociation					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Unlimited (SAR)	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Daniel M. Neumark
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code) (510) 642-3502

1. FINAL TECHNICAL REPORT

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TITLE: Spectroscopy and Dynamics of Transient and Energetic Species

DATE: 2/1/2006-1/31/2009

GRANT #: FA9550-06-1-0085

AFOSR PROGRAM MANAGER: Dr. Michael R. Berman

20090526376

2. OBJECTIVES

(unchanged)

3. STATUS OF EFFORT

Our research effort over the last three years has focused on three areas. First, we significantly improved our SEVI instrument and can now routinely obtain high resolution (0.1 – 1 meV) photoelectron spectra of negative ions, thereby obtaining new insights into vibronic coupling and other non-adiabatic effects in the open-shell neutral species generated by photodetachment. We have applied SEVI to the study of several radicals (CH_3O , propynyl, C_2H) and the pre-reactive $\text{Cl}\cdot\text{H}_2$ complex. The latter study was particularly notable as it went a long way toward settling some of the outstanding issues regarding the benchmark $\text{Cl} + \text{H}_2$ reaction. Secondly, using the widely tunable Free Electron Laser for Infrared eXperiments, FELIX, we measured the infrared spectra of hydrated sulfate dianions, $\text{SO}_4^{2-}(\text{H}_2\text{O})_n$, with as many as 24 water molecules, as well as the IR spectra of water cluster anions $(\text{H}_2\text{O})_n^-$, for clusters comprising as large as $n=50$. The sulfate work represented the first gas phase IR spectra of any multiply charged anion, and the $(\text{H}_2\text{O})_n^-$ spectra provided new insights into how excess electrons bind to large water clusters. Finally, we investigated the ultraviolet photodissociation dynamics of ClN_3 at 248 and 193 nm in order to test the effect of excitation wavelength on the product branching ratio and the possible production of cyclic N_3 .

4. ACCOMPLISHMENTS/NEW FINDINGS

A. *Slow electron velocity-map imaging (SEVI) of negative ions*

SEVI is a photodetachment technique based on photoelectron imaging aimed at detecting slow electrons at high resolution.¹ Fig. 1 illustrates the principle of the method and a comparison with two other photodetachment techniques, time-of-flight photoelectron (TOF-PE) spectroscopy and anion zero electron kinetic energy (ZEKE) spectroscopy. In anion TOF-PE spectroscopy,² mass-selected anions are photodetached with a pulsed, fixed-frequency laser, and the resulting electron kinetic energy distribution is analyzed via TOF. The energy resolution of 8-10 meV is sufficient to resolve vibrational structure for molecules and clusters that do not exhibit vibrational activity in multiple low-frequency modes upon photodetachment. Anion ZEKE spectroscopy³ yields considerably higher resolution, 1-3 cm^{-1} (0.1-0.3 meV). In this experiment,

one photodetaches with a tunable laser and collects near zero-energy electrons as a function of laser frequency. Anion ZEKE spectroscopy has produced well-resolved spectra for radicals,⁴ clusters,⁵ and transition state species,⁶ but the method is experimentally challenging and can only be applied to clusters that detach via an *s*-wave (photoelectron angular momentum $l=0$) near threshold.

In SEVI spectroscopy, one uses velocity-map imaging (VMI)⁷ to obtain photoelectron spectra at a resolution as high as $2\text{-}3\text{ cm}^{-1}$ over a relatively narrow eKE window, typically 10-100 meV. By tuning the photodetachment laser over a set of discrete frequencies, one obtains a complete, high resolution PE spectrum. SEVI offers resolution comparable to that of anion ZEKE spectroscopy, but data collection is faster by about two orders of magnitude. Moreover, SEVI is not restricted to *s*-wave detachment.

A schematic of the instrument is shown in Fig.

2. Ions are generated in a pulsed molecular beam coupled to a pulsed ionizer, mass selected by time-of-flight, and photodetached with a tunable dye laser. The resulting photoelectron is collected and imaged onto a microchannel plate detector coupled to a phosphor screen. VMI is done using

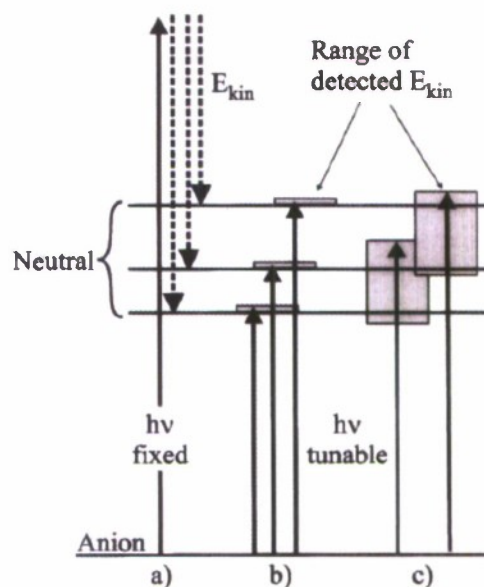


Fig. 1. Comparison of SEVI (c) with photoelectron spectroscopy (a) and anion ZEKE spectroscopy (b)

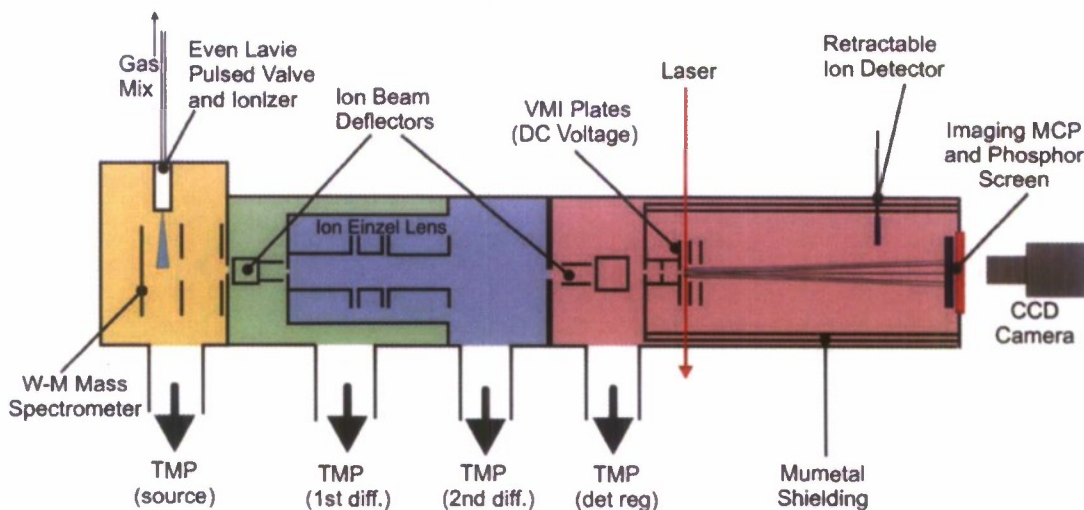


Fig. 2. Schematic of anion SEVI spectrometer.

relatively low extraction voltages (150-250 V) in order to magnify the image of low energy electrons at the detector. Over the last three years, we have optimized the performance of the spectrometer and have applied SEVI to several radicals and pre-reactive complexes, in each case resolving many new features that were not seen previously in anion PE spectroscopy.

For example, the SEVI spectrum of the methoxide anion, CH_3O^- , probed Jahn-Teller and spin-orbit coupling in the \tilde{X}^2E state of the methoxy radical, $\text{CH}_3\text{O}^\bullet$.⁸ Previous studies of CH_3O^- by anion PE spectroscopy⁹ yielded progressions assigned to the ν_5 and ν_6 degenerate vibrational modes of the radical that were allowed only because of Jahn-Teller coupling, with no discernible contributions from the totally symmetric modes that typically dominate PE spectra. The SEVI spectrum resolved several of the peaks in the PE spectrum as doublets split by spin-orbit coupling, and revealed previously unseen, weak transitions in the totally symmetric ν_2 and ν_3 modes that lay between stronger transitions in the dominant modes. In addition, several hot and sequence bands were observed for the first time, yield new vibrational frequencies for the anion.

We also measured the SEVI spectrum of the propynyl anion as a means of characterizing the 1-propynyl radical, $\text{C}\equiv\text{C}-\text{CH}_3$.¹⁰ This study represents an example of using negative ion photodetachment to investigate a high-energy neutral species; the propynyl radical lies 42 kcal/mole above the propargyl radical, $\text{H}-\text{C}=\text{C}=\text{CH}_2$, which is the lowest-energy C_3H_3 isomer.¹¹ As a result, the propynyl radical has been difficult to characterize spectroscopically. However, Lineberger and co-workers¹² showed that this species could be generated by photodetachment of the propynyl anion, which is approximately isocnergetic with the propargyl anion. While Lineberger was able to measure a vibrationally resolved PE spectrum of the anion, the features were not assigned and there was some uncertainty as to whether the radical had a 2E or 2A_1 ground state.¹³ Our SEVI spectrum revealed considerably more vibrational structure and even some rotational structure. Comparison with electronic structure calculations showed that propynyl has a 2A_1 ground state, and that pseudo-Jahn-Teller coupling with the low-lying 2E excited state is weak or non-existent.

In contrast, the C_2H radical exhibits strong vibronic coupling between its $\tilde{X}^2\Sigma^+$ and $\tilde{A}^2\Pi$ states. These states are separated by about 3700 cm^{-1} and coupled through the bend vibration (π symmetry).^{14,15} In the anion PE spectrum, this coupling appears as nominally

forbidden transitions to bend-excited levels of the neutral $\tilde{X}^2\Sigma^+$ state,¹⁶ and an extremely complex spectrum for the $\tilde{A}^2\Pi$ state that was challenging to assign because so many of the peaks were suspected to comprise overlapping transitions.¹⁷ However, in the SEVI spectrum of C_2H^- , many of these peaks were easily resolved into multiple transitions.¹⁸ Nearly all of this newly observed structure could be assigned based on comparison with high level calculations¹⁵ in which vibronic coupling between the two states was accounted for. Moreover, this was the first system for which we definitively observed *p*-wave photodetachment in the SEVI spectrum, a testament to the sensitivity of the experiment since the cross section for *p*-wave detachment is considerably less than that for *s*-wave detachment near threshold.¹⁹

Finally, we measured SEVI spectra of ClH_2^- and ClD_2^- in order to probe the pre-reactive $\text{Cl}\cdot\text{H}_2$ van der Waals (vdW) region on the potential energy surface of the $\text{Cl} + \text{H}_2$ reaction.²⁰ The purpose of this experiment was twofold. First, a study of the $\text{Cl} + \text{HD}$ reaction by Skouteris *et al.*²¹ provided experimental evidence that vdW forces in the reactant valley have a significant effect on the branching ratio of the $\text{HCl}:\text{DCl}$ product as a function of collision energy. Secondly, experiments by Liu and co-workers²² on the $\text{Cl} + \text{H}_2$ reaction suggested that the $\text{Cl}^*(^2\text{P}_{1/2})$ excited state was more reactive than the $\text{Cl}(^2\text{P}_{3/2})$ ground state. This result is at odds with expectations based on the Born-Oppenheimer approximation, since the $\text{Cl}^* + \text{H}_2$ reactants do not correlate with ground state $\text{H} + \text{HCl}$ products, and also with state-of-the-art scattering calculations.²³ It could only be correct in the presence of strong non-adiabatic

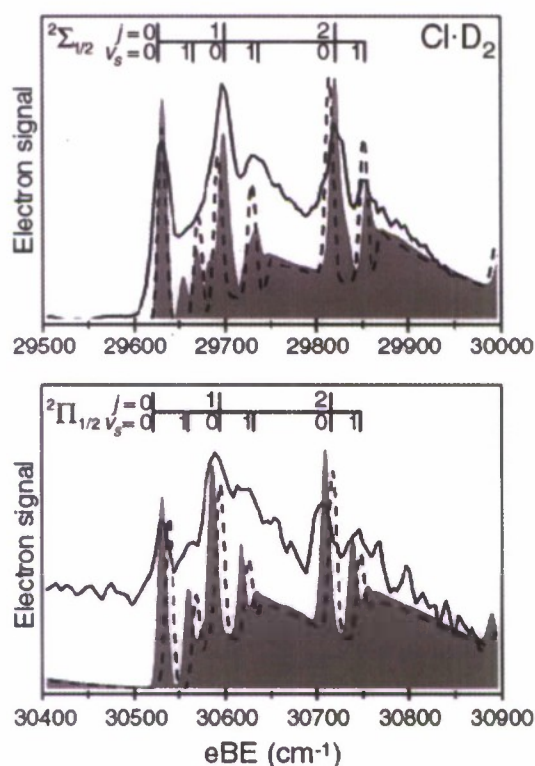


Fig. 3. SEVI spectra of ClD_2^- and comparison with adiabatic (dashed) and non-adiabatic (grey shaded) simulations. Upper and lower spectra correspond to Cl and Cl^* , respectively

coupling between the ground and excited spin-orbit surfaces in the vicinity of the pre-reactive vdW well, and such coupling would be probed by the anion SEVI spectrum.

The SEVI spectra, shown in Fig. 3, revealed progressions in low-frequency Cl·H₂ and Cl·D₂ bending and stretching modes, in contrast to the PE spectrum,²⁴ which showed no vibrational structure, and an earlier SEVI spectrum¹ that showed only partial resolution of the relatively high frequency bend modes. Fig. 3 compares the experiment to simulations with and without non-adiabatic couplings between the Cl spin-orbit states. Though non-adiabatic effects are small, their inclusion improves agreement with experiment. This comparison validates the theoretical treatment, especially of the non-adiabatic effects, in this critical region of the Cl + H₂ reaction, and shows that these effects are minor.

B. *Infrared spectroscopy of hydrated sulfate dianions and water cluster anions*

We have measured the infrared spectra, shown in Fig. 4, of gas phase, hydrated sulfate dianions, SO₄²⁻(H₂O)_n, with *n*=3-24, in order to understand the evolution of hydrogen-bonding motifs in the stepwise hydration of a dianion and to see how these motifs differ from those in the hydration of singly-charged anions.²⁵ This study was motivated by previously reported photoelectron spectra²⁶ of SO₄²⁻(H₂O)_n clusters that suggested novel water binding arrangements not present in the hydration of singly-charged anions. The experiments were performed in collaboration with Dr. Knut Asmis using the broadly tunable infrared free electron laser FELIX. A novel feature in these experiments is that mass-selected anions were trapped and cooled by collisions with He buffer gas at 18 K prior to spectroscopic investigation, thereby mitigating the uncertainty in temperature that often arises in cluster spectroscopy. Our experiments represent the first IR spectra of multiply-charged anions in the gas phase.

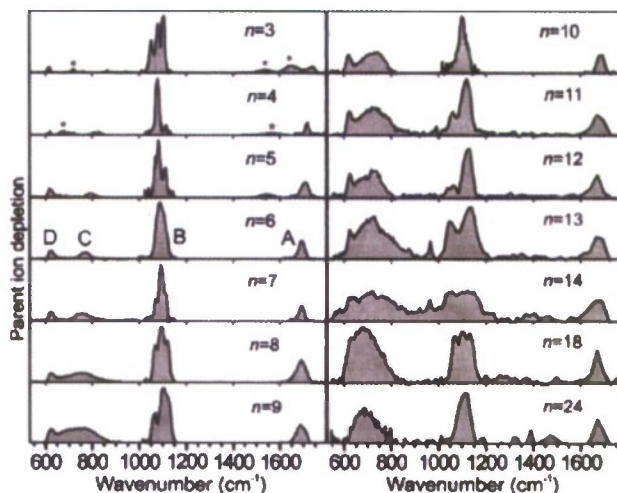


Fig. 4. Infrared spectra of SO₄²⁻(H₂O)_n anions.

The spectra showed four main bands assigned to two vibrations of the dianionic core, the water bending mode, and solvent libration. The triply degenerate SO_4^{2-} antisymmetric stretch vibration around 1100 cm^{-1} probed the local solvent symmetry; this band appeared as a singlet, doublet, or triplet, depending on the number of water molecules and the symmetry of the solvent network with respect to the sulfate chromophore. The solvent librational band, around 700 cm^{-1} , was also sensitive to the solvent hydrogen bonding network, particularly to whether hydrogen-bonding occurs solely between water molecules and the sulfate, as appears to be the case for $n \leq 6$, or if instead some hydrogen-bonding occurs between water molecules, which we believe is the case for larger clusters. The spectra and accompanying electronic structure calculations indicated a highly symmetric structure for the $n=6$ cluster, in which each water bridges two O atoms on the sulfate core, and closure of the first solvation shell at $n=12$. Our results have stimulated further experimental²⁷ and theoretical²⁸ work aimed at gaining a deeper understanding of these hydrated dianions.

Similar studies were carried out for water cluster anions $(\text{H}_2\text{O})_n^-$, $n=15-50$,²⁹ with the goal of (a) determining the electron binding motif over a larger size than had been previously investigated³⁰ and (b) testing the effect of cooling on the IR spectra of these clusters. Signal was seen in two frequency regions centered around 700 and $1500-1650\text{ cm}^{-1}$, corresponding to water librational and bending motions, respectively. The bending feature associated with a double-acceptor water molecule³¹ binding to the excess electron was clearly seen up to $n=35$. However, starting around $n=25$, this feature began to blue-shift and broaden, suggesting more delocalized electron binding for the larger clusters in which the excess electron interacts with multiple water molecules.

C. *Photodissociation of ClN_3*

The photodissociation dynamics of ClN_3 at 248 and 193 nm were investigated by molecular beam photofragment translational spectroscopy.³² This research was motivated by experiments by Wodtke and co-workers³³ in which ultraviolet photolysis of ClN_3 yielded a bimodal Cl atom translational energy (E_T) distribution. The energetics of the faster peak were consistent with production of $\text{Cl} + \text{linear N}_3$, while those for the slower peak appeared consistent with a high energy, cyclic isomer of N_3 predicted by Morokuma and co-workers.³⁴ In our experiments,³⁵ both the Cl and N_3 photofragments could be observed, allowing one to determine

if, indeed, each of the two component of the Cl E_T distribution could be momentum-matched to corresponding N_3 products.

The results at 248 nm are shown in Fig. 5, where we show the center-of-mass E_T distributions for Cl and N_3 products. Each distribution is bimodal. The fast peaks for both masses match very well, indicating production of Cl and stable N_3 products. However, the slower N_3 peak is truncated at $E_T < 25$ kcal/mol, while the Cl peak extends to considerably lower E_T . These results show that the slower product channel is Cl and a high energy form of N_3 that dissociates en route to the detector.

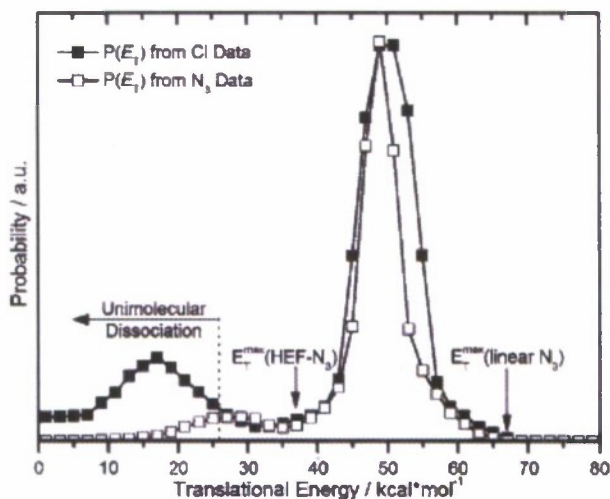


Fig. 5. Translational energy (E_T) distributions of Cl and N_3 fragments from photodissociation of ClN_3 at 248 nm.

The energetics of this dissociation are again consistent with the those of cyclic N_3 . Interestingly, at 193 nm, we again find a bimodal distribution for the Cl product, but the E_T distribution of the Cl atoms is nearly the same as at 248 nm, indicating that the additional photon energy is channeled entirely into internal energy of the N_3 fragments. As a consequence, the N_3 E_T distribution truncates at considerably higher E_T than at 248 nm. Overall, our results show that the bimodal Cl distribution is robust and that both components correlate to N_3 fragments. We cannot say from our work whether the high energy form of N_3 is in fact cyclic, but more recent experiments by Wodtke³⁶ support this assignment.

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6. PUBLICATIONS

1. M. J. Nee, A. Osterwalder, J. Zhou, and D. M. Neumark, "Slow Electron Velocity-map Imaging Photoelectron Spectra of the Methoxide Anion." *J. Chem. Phys.* **125**, 014306 (2006).
2. J. Zhou, G. Santambrogio, M. Brummer, D.T. Moore, L. Woste, G. Meijer, D. Neumark, and K. Asmis. "Infrared Spectroscopy of Hydrated Sulfate Dianions." *J. Chem Phys.* **125**, 111102. (2006).
3. D. M. Neumark. "Probing Chemical Dynamics with Negative Ions." *J. Chem. Phys.* **125**, 132303. (2006).
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12. E. Garand, T. I. Yacovitch, and D. M. Neumark. "Slow Photoelectron Velocity-map Imaging Spectroscopy of C₂N⁺, C₄N⁺ and C₆N⁺." J. Chem. Phys. 130, 064304-1. (2009).
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7. INTERACTIONS/TRANSITIONS

July 2-7, 2006

Spectroscopy and Dynamics on Multiple Surfaces

Telluride, CO

Lecture Given During Conference

July 8-13, 2007

Santa Fe, New Mexico

Dynamics of Molecular Collision (DMC) Conference

Lecture Given During Conference

December 6-11, 2007
Manchester, England
Photon Science Institute/University of Manchester, England
Lecture Given During Conference

January 26-February 1, 2008
Il Ciocco, Italy
Gordon Research Conference
Lecture Given During Conference

April 5-10, 2008
New Orleans, Louisiana
American Chemical Society Meeting
Lecture Given During Conference and Presentation Given for Irving Langmuir Award

April 28, 2008
Argonne, Illinois
Argonne National Laboratory
Lecture Given During Conference

April 29, 2008
Chicago, Illinois
Northwestern University
Lecture Given During Conference

July 27-31, 2008
Telluride, Colorado
Dynamics on Multiple Potential Energy Surfaces
Invited Lecture

August 18-20, 2008
Philadelphia, Pennsylvania
ACS National Meeting and Exposition
Invited Lecture

September 5-12, 2008
Aussais, France
Gordon Research Conference Molecular and Ionic Clusters
Dr. Neumark was Conference Chair

October 22-24, 2008
Honolulu, Hawaii
Physical Chemistry Seminar
Invited Lecture

8. NEW DISCOVERIES, INVENTIONS, OR PATENT DISCLOSURES

None.

9. HONORS/AWARDS

Irving Langmuir Award in Chemical Physics, American Chemical Society, 2008

Dudley R. Herschbach Medal, 2009